WHAT'S LACKING WITH FRACKING

THE FUEL-EXTRACTION METHOD BEHIND
THE U.S. ENERGY BOOM GETS NEW SCIENCE TO
MITIGATE WASTEWATER AND OTHER ENVIRONMENTAL
CONCERNS WHILE IMPROVING EFFICIENCY.



U.S. CARBON EMISSIONS ARE DECLINING. In the past ten years, per-capita emissions of carbon dioxide have dropped to a level not seen since the 1960s, attributed in large part to a recent surge in natural-gas production. With natural gas becoming cheap and abundant, electrical power generation has partially shifted away from coal. And because natural gas generates only about half as much carbon dioxide as coal for every watt of energy produced, the nation is putting less carbon into the atmosphere—all while stimulating the economy and raising the possibility of U.S. energy independence.

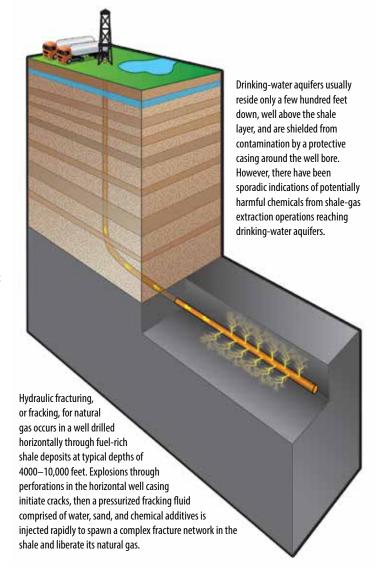
The trouble is, most of this natural gas has been coming from shale formations more than a mile underground, and there are distinct technical and environmental challenges associated with getting it out. Currently, such operations extract only about 15 percent of the natural gas in place and annually consume about a hundred billion gallons of freshwater to do so, turning much of it into highly toxic wastewater too expensive to remediate. The wastewater is usually re-injected deep underground, just to get rid of it. But both the fuel extraction and wastewater reinjection create the risk that toxic fluids could migrate along defective wellbores, or natural faults and fractures, into drinking-water aquifers. In addition, wastewater reinjection has been shown to cause low-level earthquakes. By increasing the pressure in subsurface pores, the process can increase seismicity in regions with stressed, preexisting faults.

Not surprisingly then, the most successful method of shale-gas extraction, known as hydraulic fracturing, or fracking, is fraught with controversy. Even the most cursory of internet searches on the term instantly reveals a flurry of opposition—and opposition to the opposition. The controversy, however, is somewhat misplaced.

fracking operations typically leave 80-90% of the available fuel in the ground.

"Fracking itself is not the problem," says Los Alamos earth and environmental scientist Hari Viswanathan. "That deep underground, the fractures don't extend far enough upward to penetrate drinking-water aquifers. It's the large-scale industrial operations at the surface, the potential leakage paths formed by wells, and the disposal of wastewater that create the problems."

Viswanathan leads a multidisciplinary team of expert scientists, postdoctoral researchers, and students in a broad effort to develop the interconnected science—the mechanics, chemistry, thermodynamics, and hydrodynamics on scales ranging from nanometers to kilometers—of how fracturing really affects the deep geological formations. His hope is that it will lead to better environmental security, in terms of subsurface oil and gas movement, and substantially more efficient extraction of shale gas. That would mean fewer wells producing more gas per well, which would lower the overall



water use, lower the wastewater injection and associated earthquakes, and lower the risk of groundwater contamination—all while obtaining more of a relatively clean-burning fuel.

How fracking works

"Hydraulic fracturing for shale gas is a clever way to extract what has long been an inaccessible resource," Viswanathan says. "You can't just draw it up because the gas is trapped inside a low-permeability rock. Nothing flows from it."

The solution in use today involves a number of innovations, beginning with a very deep well that drops straight down and then slowly arcs to run horizontally through the heart of the shale layer. Explosive charges along the horizontal section create perforations through the well casing and cut into the shale formation. Then a pressurized mixture of water, sand, and chemicals is injected in a rush to frack the rock, generating a rich network of fractures. If the process is successful, fuel will be able to move through the fractures.

Lowering the pressure at the well head generates suction that may lead to years of natural gas production, as long as the fractures remain open. However, these shale formations often reside 8000 feet below the surface, and the weight of all that overlying rock tends to squeeze the fractures closed again. That's why sand is included in the fracking fluid. The sand is selected to have an ideal grain size for propping open the fractures once they have been created and, for that reason, is referred to as a proppant, or propping agent.

In addition to the proppant, chemical additives are included in the fracking fluid. Biocides prevent microbial activity, and soapy surfactants reduce the fluid's viscosity, allowing more energy to be delivered to the fracture tips for a better fracture network overall. Unfortunately, the use of these chemicals, some cancer causing, also introduces the danger that they might find their way into drinking-water aquifers. Indeed, an Environmental Protection Agency (EPA) report out earlier this year finds examples of drinking-water contamination due to fracking operations, stemming both from surface spills and fluid migration along defective wellbores. Yet the report shows that the contamination identified so far is quite limited and finds no "widespread, systemic impacts on drinking water resources in the United States."

As Viswanathan explains, chemical additives shouldn't be considered the only source of contamination risk anyway, regardless of their movement underground, because the toxin-infused fluid drawn back up from the well is generally worse than the chemicals that were sent down. Fracking water withdrawn during the well's productive life contains large quantities of naturally occurring salts, heavy metals, and radioactive elements from deep underground, in addition to the original additives. So the objective of protecting the environment, as Viswanathan sees it, shouldn't just be about reducing additives; it should be about reducing water use altogether.

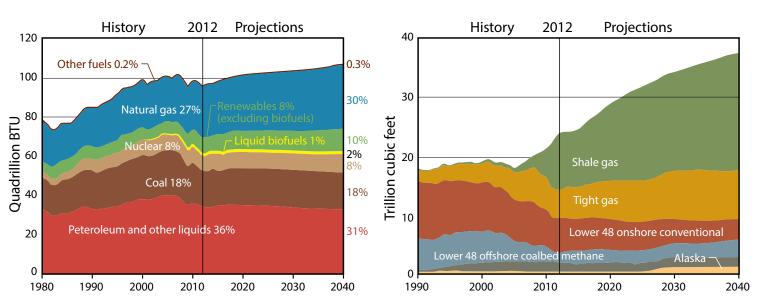
Sweep and scour

Deep-shale deposits are a compressed blend of finegrained rock, natural gas, and hydrocarbon oil (also valuable). Neither the oil nor the gas generally resides within large open holes in the rock; rather, they occupy naturally existing fractures and tiny pores. They also exist in a form chemically adsorbed to other organic molecules in the rock.

Ideally, fracking operations tap into all of these locations. First, fracking-induced fractures link to existing fractures and access the fuel from them; this is the low-hanging fruit of the fuel-from-shale world. Once the fuel is drawn from the in-place fractures accessed by the initial fracking, it might then be drawn from an extensive network of mechanically damaged rock surrounding the primary fracture network. Then hopefully the fracture-damage zone allows the fracking fluid to sweep through to access small pores and, when drawn back out, gather their fuels. Over longer periods of time, the fluid could desorb fuels attached to solid organic matter and pull those out as well.

This idealized progression seems consistent with industry experience. Fuel production dwindles rapidly during the first few years, presumably as larger, existing fractures are drained, and smaller pockets feed the well more slowly. Nonetheless, in the end, fracking operations typically leave 80–90 percent of the available fuel in the ground. In some cases, oil and gas operators may be able to get more fuel out by refracking an existing well after a few years. But the gas recovery remains inefficient overall, and a significant reason for that turns out to be the fracking water itself.

When water is injected to frack a well, the desirable outcome of establishing fractures is accompanied by two undesirable outcomes, which may inhibit access to all but the most easily accessed fuel within the shale. First, the shale rapidly soaks up most of the water like a sponge, causing it to swell and therefore closing the fractures, both natural and man-made. Second, water fills in the fractures, effectively sealing off the fuel inside because of water's high surface tension and the fact that it doesn't mix with hydrocarbon fuels (like oil). Both inhibiting effects are more pronounced in the smaller fractures within the network and could be minimized by choosing another fluid instead of water.

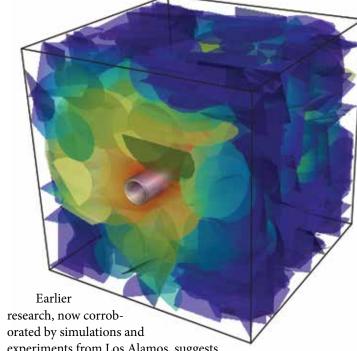


(Left) In 1990, natural gas made up 23 percent of American energy consumption, but that share has been rising, partially displacing coal and petroleum in recent years. By 2012, natural gas made up 27 percent of American energy consumption and is projected to reach 30 percent by 2040. (Right) Shale gas, mostly from fracking, was a negligible source of natural gas in 1990 but by 2012 exceeded all other individual sources and is projected to exceed all other sources combined by 2040.

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CREDIT: Energy Information Administration

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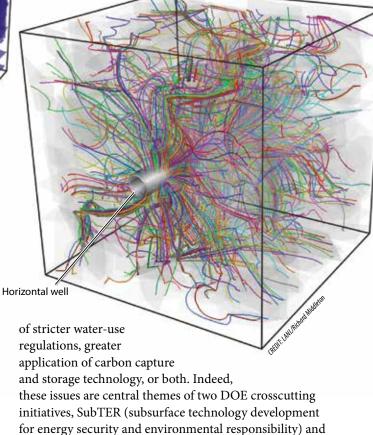
experiments from Los Alamos, suggests that a fluid based on supercritical carbon dioxide (scCO₂), with attributes of both gas and liquid, could prove more effective in a variety of ways. Initially, it may be able to produce a more elaborate and extensive fracture network than water because when it expands into a new volume, it cools like gas expanding from a spray can, and thereby generates thermally induced fractures. That means an scCO₂ fracking fluid should generate more fractures than water as it moves through the shale. More research is needed to confirm this—and don't worry, Viswanathan is working on it—but even if water initiates the fracking and remains in place, scCO₂ can still be used in a secondary process, moving through the water to help extract the fuel.

Compared to water, $scCO_2$ also has less of a flow-blocking effect due to its lower surface tension and its miscibility with hydrocarbons. Natural gas in pockets trapped by water would instead dissolve into $scCO_2$. And $scCO_2$ even displaces chemical bonds that cause natural gas molecules to adhere to organic matter in the shale. Effectively, it sweeps the fuel from inside the fracture network and scours it from the walls. Perhaps more important still, its use could greatly reduce (or even eliminate) the need for risky chemical additives and greatly reduce (or even eliminate) the production of toxic wastewater that is currently re-injected underground. And if the $scCO_2$ must be re-injected, that solves another problem by keeping it out of the atmosphere.

On its own or mixed with water, scCO₂ has been used in oil and gas drilling in the past and is sometimes used today to extract more gas than water alone. Results have been inconsistent at times, but in previous experiments sponsored by the Department of Energy (DOE), the use of scCO₂ has increased natural gas production by up to five times over water alone while dramatically cutting water consumption.

So why is water still the fluid of choice? The simple answer is price. Right now, water, even drinking-quality water, is much less expensive than scCO₂ in the quantities needed for fracking operations. However, that may change in the face

High-performance computing simulation of fracking-well operations: (Above-left) Slivers represent existing cracks in the shale that harbor natural gas and other hydrocarbon fuels. Fracking produces additional fractures, extending outward from the horizontal well. The man-made fractures intersect with existing cracks and create a path for fuel to flow into the well, and an applied pressure gradient (indicated by color) drives the flow. (Below-right) Hundreds of fuel-flow trajectories are identified, allowing researchers to compute the natural-gas production rate over time.



"I think we are on our way toward demonstrating an economics of natural gas production that actually favors smaller environmental impacts," says Viswanathan. "We just need realistic calculations—and experiments carried out under realistic conditions to validate them—to show us the way there."

the Water-Energy Nexus (interdependence between water

and energy resources). But even under existing water and

carbon regulations, the price-motivated choice of water for

capability that allows natural gas companies to recover the

fracking could change in the face of a new scientific prediction

lion's share of the fuel left in place by their current operations.

Crack team

Satish Karra, Esteban Rougier, Mark Porter, and Robert Currier are fluid flow, rock mechanics, and chemistry researchers on Viswanathan's team. They are responsible for crafting a detailed computer simulation of fractured natural-gas systems deep underground and generating critical experimental data to feed into it. The idea is, if the simulation accounts for all the relevant processes, then it can answer all the what-if questions one might ask to work out the best way to obtain the most natural gas with the least environmental

risk. What if we apply X amount of pressure and cycle it up and down? What if we use a 60–40 mixture of water and scCO $_2$? What if we change proppants and maybe re-frack periodically?

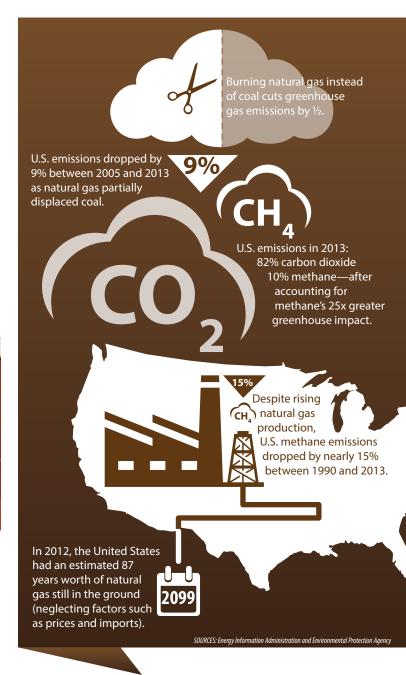
The simulation is complex because it must take into account a variety of physical processes occurring across an enormous range of size scales. Karra, for example, has focused heavily on the scale of the overall shale reservoir, analyzed over the kilometers surrounding the well site. Rougier, by contrast, studies the core scale, ranging from a hundred-thousandth of a meter up to several meters and representing fracking features in the immediate vicinity of the well. Porter examines other scales that extend much smaller, to millionths and even billionths of a meter, representing micro-fractures and tiny natural pores in the shale, respectively. Each scale corresponds to a different set of key processes—e.g., fracture propagation at the core scale and multiphase fluid dynamics at the micro-scale—and all of this must feed into the simulation for accurate results.

Karra begins with a model of the reservoir geology surrounding a horizontally drilled well. He programs his simulation to include a number of simplified, preexisting planar fractures at various angles within the shale. He then simulates the effect of fracking by establishing new fractures that extend radially outward at regularly spaced intervals along the well. These man-made fractures intersect the preexisting, natural ones and thereby access the natural gas trapped within them. To simulate drawing the gas out, he creates a pressure gradient and, by taking into account pressure, aperture, and porosity effects, calculates flow rates and predicts natural-gas production over the operational life of the well. But unlike existing computer models already in use by industry, which tend to rely on overly idealized conceptions of the reservoir or simply impose the observed outcomes from other well sites, Karra's simulation is built upon first-principle, computational physics grounded by reliable fracture datasets to guide the core-scale activity.

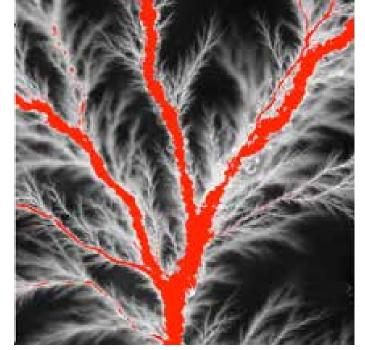
X-ray computed tomography image (left) and computer simulation (right) of fracturing produced by applying a shear force (red arrows) to an industry core sample of drilled shale. The experiment is carried out in a containment vessel at high temperature and pressure conditions, representative of those occurring in deep-shale deposits. Since the pressure exerts a force from all sides, in all three dimensions, researchers call this a triaxial experiment. X-ray imagery like this is used to improve the accuracy of the simulation to better predict shale fracturing under different conditions.

These reliable fracture datasets have to come from somewhere, and that's where Bill Carey, a Los Alamos oil-andgas expert, comes in. Carey begins with a cylindrical core sample of shale, 1–3 inches long and 1 inch in diameter, provided by industry partner Chesapeake Energy. Then he subjects it to three-dimensional stresses in what's called a triaxial experiment to induce realistic hydraulic and shear fracturing within the sample. He has pioneered a unique capability to accomplish this within a high-temperature, high-pressure containment vessel housed inside an x-ray computed tomography system to observe fracturing directly at the actual conditions found in deep-shale reservoirs, including how the shale soaks up water.

Rougier uses these fracture-experiment results to calibrate a core-scale, finite-element computer simulation of the process. When the simulation correctly produces a nearly identical fracture network from the same stresses imposed on the



More about **natural gas** 29



Oil (shown in red) being pushed into a laboratory-synthesized fracture network floods large channels but does not reach into dead-end extremities, implying that relevant fluid behaviors like capillary action and surface tension cannot be ignored when predicting flow in and out of the large number of small fractures.

physical sample, Rougier knows he's got the fracture physics right. Then his simulation can be used to predict fracture propagation under different fluid compositions, rock characteristics, and injection schemes.

In addition, Carey measures the permeability of the sample—still in the pressurized experimental apparatus—from which he and Rougier can calculate fuel extraction rates. As expected, the measured permeability is zero until fractures form, then spikes up and diminishes with time as the unrelenting pressure squeezes the fissures closed. These permeability results, too, are incorporated into the core-scale computer simulation, and the core-scale simulation is incorporated into the reservoir-scale simulation. All together, the simulation correctly reproduces the production curve—depicting natural-gas extraction over time—obtained from industry experience. The curve climbs rapidly upon initial fracturing and drops away as the permeability declines over the following years. However, the simulated curve shows less production than what actually occurs in the later years.

"Our simulation doesn't yet include the micro- and nano-scale effects that govern natural-gas production after the larger pockets have been emptied," explains Viswanathan. "We need data to characterize that as well."

The little things

Porter, Currier, and Carey are addressing that objective with a series of microfluidics experiments, which are just what they sound like: fluid-flow tests using tiny channels, representing the channels where much of the shale gas is trapped. The data they obtain will be merged into the overall simulation to better explain production in later years and provide a more complete basis for assessing the likely impacts of various proposed improvements to the process.

In a simple initial experiment, Porter and Currier created an idealized fishbone-patterned fracture network in a microfluidic wafer made of shale. They saturated it with oil and then drove water through it with a pressure gradient along its spine. The water did not penetrate into the side channels and therefore demonstrated its inability to sweep out hydrocarbon fuels from dead-end fractures. The team also made an advanced fluid-dynamical computer model of the same setup and verified its ability to match the results of the experiment, including the detailed shape of the water "finger" making its way through the oil.

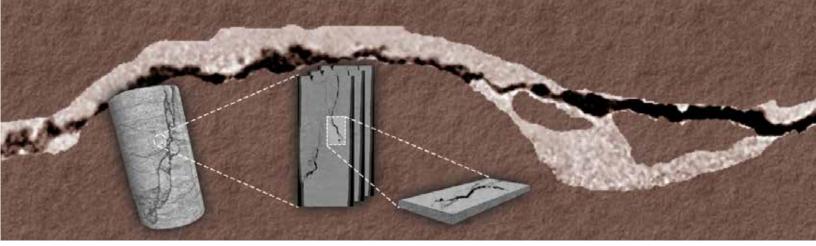
But realistic fractures are better than idealized ones, so Porter, Currier, and Carey perform sophisticated x-ray and neutron tomography on the fractured samples from the triaxial experiments and, using the resulting imagery as a guide, etch their actual fracture patterns into microfluidic shale wafers. Then they push different fluids through, including oil, water, and scCO₂.

When they tried pushing oil through a complex fracture network, the oil didn't reach the network's narrow, dead-end extremities due to micro-scale fluid-physics effects: surface tension, capillary forces, wetting properties of the rocks, and the like. These are evidently very important at small scales. And when they tried injecting water followed by scCO₂ into a real fracture network etched in shale, they observed the scCO₂ tunneling through the water in a distinctive fashion, demonstrating that the different fluids have very different capabilities within fractured shale. Discoveries from microfluidics experiments like these, together with other results on even smaller scales, will be added to the overall multiscale permeability calculation within the reservoir-scale fracking simulation.

We may discover an economics of natural-gas production that actually favors smaller environmental impacts.

"The science of hydraulic fracturing for hydrocarbon fuel is surprisingly difficult to uncover," says Viswanathan. "It's tremendously important, for example, that we've learned how to carry out our experiments, both fracturing and microfluidics, under actual reservoir temperatures and pressures. The fluid and wetting properties that dominate the fuel-sweep interactions depend greatly upon those temperatures and pressures. And as for $scCO_2$ "—he spells out the letters rather than voicing 'supercritical carbon dioxide'—"well, SCO_2 wouldn't even be so without the high T and P."

It was no easy task to conduct realistic experiments at actual reservoir conditions; it took nearly five years to develop the necessary techniques, combining a variety of disparate Los Alamos capabilities from well beyond Viswanathan's Earth Sciences office suite—capabilities like high-performance computing, neutron tomography at the Los Alamos Neutron



Fractures produced in real shale during triaxial experiments (see image on page 29) and revealed by microtomography are etched into shale wafers for microfluidics experimentation. Here, water (gray-tan) fills a fracture, and subsequently injected supercritical carbon dioxide (black) displaces its way through the water to access potential natural-gas pockets. Alternate fluids like supercritical carbon dioxide may prove more efficient and more environmentally friendly than water if they can be made cost effective.

Science Center, and microscopic etching at the Lab's Center for Integrated Nanotechnologies. But now, after a decade of groundwork (so to speak), he is ready to get some answers: how water hinders fuel extraction, whether alternative fluids can deliver better performance or reduced swelling, and what the overall permeability of fractured shale is. His team is at the forefront of all these things.

Subsurface crossroads

The shale-gas industry has been slowly improving its extraction efficiencies—getting more gas out—by brute force, drilling longer horizontal wells and placing more fracture-initiation stages along their length. But Viswanathan says there is a sentiment in the field that these sorts of improvements have already maxed out. It is only through a genuine quantitative science of fracking that further improvements of any real significance are likely to materialize.

That same new science also appears to be the nation's best near-term hope for mitigating environmental dangers while reducing carbon emissions from burning coal. A substantial

Hari Viswanathan inspects a microfluidic cell used to study the extraction of hydrocarbon fuels from a complex (and in this case, synthetic) fracture network.

reduction in fracking water use (and therefore wastewater production) is unlikely until better knowledge is available to inform alternate-fluid practices and higher-efficiency extraction strategies. And more reliable containment of fracking-well toxins, protection of drinking-water aquifers, and even safeguards against atmospheric leaks are unlikely without a more developed science of fracture generation and propagation. (Pound for pound over a 100-year period, natural gas is 25 times more potent than carbon dioxide as a greenhouse gas, according to the EPA. It would be a shame to ruin the lower carbon-emission rates achieved in recent years because of gas leaks reaching the surface.)

Unknowns remain, of course. Small-scale effects have yet to be fully accounted for in Viswanathan's simulations, and different fracturing methods—using still other fracking fluids, such as nitrogen, or none at all and explosives instead—have yet to be sufficiently studied. In addition, his new subsurface science has yet to be repackaged in earnest for other energy contexts beyond fossil-fuel extraction, such as carbon capture and storage, geothermal energy, and underground nuclearwaste repositories. But the potential to advance each of these energy applications is definitely there, as is the remarkable potential for national energy independence.

With so much riding on a science-based predictive capability for deep drilling, there's no question: when it comes to establishing the science and putting it to use, it's time to get cracking. LDRD

—Craig Tyler

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